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*Acta Cryst.* (2008). F**64**, 686-691 [ doi:10.1107/S1744309108019623 ]

## Structure of the *Brachydanio rerio* Polo-like kinase 1 (Plk1) catalytic domain in complex with an extended inhibitor targeting the adaptive pocket of the enzyme

**R. A. Elling, R. V. Fucini, E. J. Hanan, K. J. Barr, J. Zhu, K. Paulvannan, W. Yang and M. J. Romanowski**

**Abstract:** Polo-like kinase 1 (Plk1) is a member of the Polo-like kinase family of serine/threonine kinases involved in the regulation of cell-cycle progression and cytokinesis and is an attractive target for the development of anticancer therapeutics. The catalytic domain of this enzyme shares significant primary amino-acid homology and structural similarity with another mitotic kinase, Aurora A. While screening an Aurora A library of ATP-competitive compounds, a urea-containing inhibitor with low affinity for mouse Aurora A but with submicromolar potency for human and zebrafish Plk1 (hPlk1 and zPlk1, respectively) was identified. A crystal structure of the zebrafish Plk1 kinase domain-inhibitor complex reveals that the small molecule occupies the purine pocket and extends past the catalytic lysine into the adaptive region of the active site. Analysis of the structures of this protein-inhibitor complex and of similar small molecules cocrystallized with other kinases facilitates understanding of the specificity of the inhibitor for Plk1 and documents for the first time that Plk1 can accommodate extended ATP-competitive compounds that project toward the adaptive pocket and help the enzyme order its activation segment.

PDB reference: 3db6

**Keywords: Polo-like kinase 1; small-molecule inhibitors; zebrafish.**

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*Acta Cryst.* (2008). D**64**, 339-353 [ doi:10.1107/S0907444907068217 ]

## Structure of wild-type Plk-1 kinase domain in complex with a selective DARPin

**T. M. Bandeiras, R. C. Hillig, P. M. Matias, U. Eberspaecher, J. Fanghänel, M. Thomaz, S. Miranda, K. Crusius, V. Pütter, P. Amstutz, M. Gulotti-Georgieva, H. K. Binz, C. Holz, A. A. P. Schmitz, C. Lang, P. Donner, U. Egner, M. A. Carrondo and B. Müller-Tiemann**

**Abstract:** As a key regulator of mitosis, the Ser/Thr protein polo-like kinase-1 (Plk-1) is a well validated drug target in cancer therapy. In order to enable structure-guided drug design, determination of the crystal structure of the kinase domain of Plk-1 was attempted. Using a multi-parallel cloning and expression approach, a set of length variants were identified which could be expressed in large amounts from insect cells and which could be purified to high purity. However, all attempts to crystallize these constructs failed. Crystals were ultimately obtained by generating designed ankyrin-repeat proteins (DARPins) selective for Plk-1 and using them for cocrystallization. Here, the first crystal structure of the kinase domain of wild-type apo Plk-1, in complex with DARPin 3H10, is presented, underlining the power of selective DARPins as crystallization tools. The structure was refined to 2.3 Å resolution and shows the active conformation of Plk-1. It broadens the basis for modelling and cocrystallization studies for drug design. The binding epitope of 3H10 is rich in arginine, glutamine and lysine residues, suggesting that the DARPin enabled crystallization by masking a surface patch which is unfavourable for crystal contact formation. Based on the packing observed in the crystal, a truncated DARPin variant was designed which showed improved binding characteristics.

PDB reference: 2v5q

**Keywords: protein kinase; multi-parallel expression and purification; isothermal titration calorimetry; surface-entropy mutation; structure-guided drug design; ribosome display.**

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*Acta Cryst.* (2008). D**64**, 909-918 [ doi:10.1107/S0907444908019513 ]

## Structures of the wild-type and activated catalytic domains of *Brachydanio rerio* Polo-like kinase 1 (Plk1): changes in the active-site conformation and interactions with ligands

**R. A. Elling, R. V. Fucini and M. J. Romanowski**

**Abstract:** Polo-like kinase 1 (Plk1) is a member of a family of serine/threonine kinases involved in the regulation of cell-cycle progression and cytokinesis and is an attractive target for the development of anticancer therapeutics. A zebrafish homolog of the human Plk1 (hPlk1) kinase domain (KD) was identified that can be expressed in large quantities in bacteria and crystallizes readily, whether in a wild-type form or as a variant containing the activating Thr196→Asp substitution, in one space group

and under similar conditions both in the absence and presence of active-site compounds. This construct was validated by testing a panel of hPlk1 inhibitors against human and zebrafish proteins and it was shown that the selected small molecules inhibited the homologs with a high degree of correlation. Crystal structures of ligand-free wild-type and activated zebrafish Plk1 (zPlk1) KDs revealed the organization of the secondary structural elements around the active site and demonstrated that the activation segment was disordered in the activated form of the domain but possessed a well defined secondary structure in the wild-type enzyme. The cocrystal structure of wild-type zPlk1 KD with ADP documented the hydrolysis of ATP and revealed the phosphorylation site. The cocrystal structure of the activated KD with wortmannin, a covalent inhibitor of Plk1 and PI3 kinases, showed the binding mode of the small molecule to the enzyme and may facilitate the design of more potent Plk1 inhibitors. The work presented in this study establishes the zPlk1 KD as a useful tool for rapid low- and high-throughput structure-based screening and drug discovery of compounds specific for this mitotic target.

PDB references: 3d5u, 3d5v, 3d5w and 3d5x

**Keywords: Polo-like kinase 1; small-molecule inhibitors; zebrafish.**

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*Acta Cryst.* (2008). A**64**, C234

### Expression, purification and crystallization of *Aurora* kinase C

**M. Isogai, T. Kinoshita, T. Nakaniwa, A. Yamaguchi, M. Gouda, K. Yokota, H. Ishiguro and T. Tada**

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### Comparison of lysozyme structures derived from thin-film-based and classical crystals

**E. Pechkova, V. Sivozhelezov, G. Tropiano, S. Fiordoro and C. Nicolini**

**Abstract:** The present report is dedicated to a systematic comparison of crystal structures produced by the nanobiofilm template method and by the classical hanging-drop vapour-diffusion method. Crystals grown by the innovative nanostructured template method appear indeed radiation-resistant even in the presence of a third-generation highly focused beam at the European Synchrotron Radiation Facility. The implications of this finding for protein crystallography are discussed here in terms of water redistribution and of the detailed atomic resolution comparative studies of the two crystal structures with or without nanobiofilm template, as emerging also from circular-dichroism and thermal denaturation studies.

**Keywords: thin films; lysozyme.**

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### Structure and function of Survivin-Borealin-INCENP core complex in mitosis

**A. A. Jeyaprakash, U. R. Klein, E. A. Nigg and E. Conti**

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**Structural and functional studies of the probiotic organism *Lactobacillus salivarius***

**M. Bumann, H. Gut, F. Fang, P. O'Toole and M. A. Walsh**